:CHEMICAL BONDING:

Introduction:

chemical bond is basically force.

I) TYPES OF chemical bond

B.E 200-400 KJ/mole → Inter Atomic (S. bond)

- → ionic, covalent bond
- → coordinate
- → metallic

B.E → 2-40 KJ/mole → intermolecular (weak bond)

↓ blw two molecules

- → vander wall force
  - ↓
  - 5 types
- → H-Bond
  - → intermolecular
  - → intramolecular

2) cause of chemical bonding

3) Ionic Bond formation, Lattice energy
   ↓ nondirectional → structure is not

4) % of covalent character in ionic bond
   ↓
   Fajan's Rule

5) covalent bonding → Directional → structure

6) Dipole moment
   ↓
   How much ionic character in covalent bond.

7) Theories of covalent bond

VBT, VSEPR, MOT, Hybridization
↓ ↓ ↓ ↓
σ, π bond, shape, orbital in molecules, Geometry

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Cause of chemical combination: → stability

Why bond is formed?

Two theories

① To achieve octet Rule / Noble gas configuration

↓ Old theory

$ns^2 np^6 = 8\bar{e}$ in last shell

He Ne Ar Kr Xe Rn

Ne: $2s^2, 2p^6$ → $8\bar{e}$

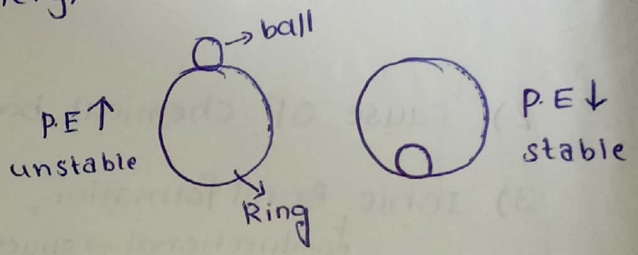
Ar: $3s^2, 3p^6$ → $8\bar{e}$

Noble gases are stable bic they have 8 ē's in last shall so every element wants to stable so he try to follow the octet Rule.

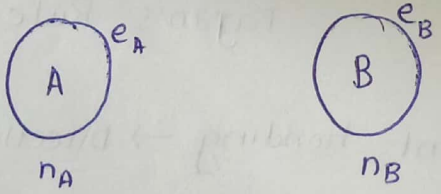
② To lower P.E OF system:

↓ New theory

stable → Energy lowest

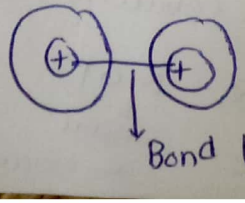


Every thing wants to lower its P.E



$n_A - n_B$, $e_A - e_B$ } Repel

$n_A - e_B$, $n_B - e_A$ } Attract



Stable ≡

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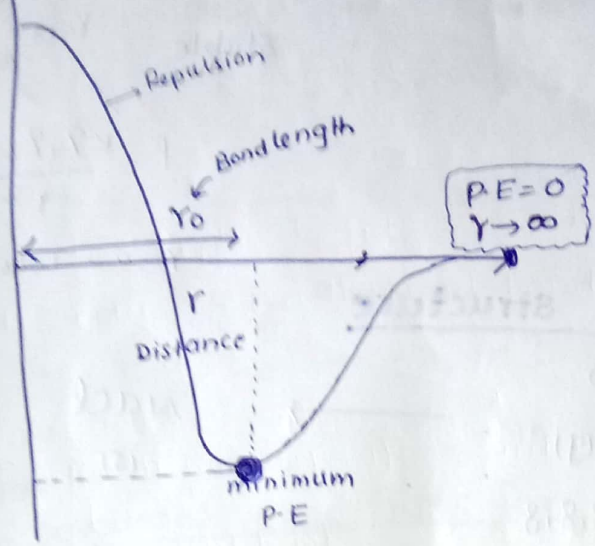

- As The distance more decrease the Repulsive forces starts thus P.E increase.

Lewis Concept (Classical Theory About chemical Bonding)

Ionic Bonding: (Electrovalent bond)

Metal + non metal

➡ here complete transfer of $\bar{e}$ occur

$$Na \longrightarrow Na^+ + \bar{e}$$
2,8,1 → 2,8

$$Cl + \bar{e} \longrightarrow Cl^{\ominus}$$
2,8,7 → 2,8,8

$Na^{\oplus} \cdots\cdots Cl^{\ominus}$

Attraction ↓ electrostatic Force of attraction.

✔ ionic bond Actually not a bond it is only force. so it is not Represented by a bond.

$Na - Cl$ ✗ $NaCl$

Na^+ (2,8) Cl^- (2,8,8)

Na^+ & Cl^- are both stable bic in last shall both have 8 $\bar{e}$'s but why they React ?

Answer: $\bar{e}$ losed by Na^+ in gaseous state

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Na^+ gaseous + Cl^- (g) ⟶ NaCl (s) → strong electro-static force of Attraction

* gaseous state ⟶ unstable

Stable

$F = \frac{KQ_1Q_2}{r^2}$

Y = v.v. low

Lewis Dot Structure

NaCl:

$Na^+_{(g)} + Cl^\ominus_{(g)} \longrightarrow NaCl_{(s)}$

2,8,— 2,8,8

Before Bond Formation

After Bond Formation

$Na^\oplus$ + $:\overset{\otimes}{Cl}:$ (⊗ from Na) OR $Na^\bullet \rightarrow :\overset{\cdot\cdot}{Cl}:$

$MgCl_2$:

$Mg_{(g)} \longrightarrow Mg^{2+}_{(g)} + 2\bar{e}$

2,8,2

$2Cl + 2\bar{e} \longrightarrow 2Cl^\ominus$

2,8,7 2,8,8

$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}:$

Lewis structure ≡ Mg^{2+} $:\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}:$ OR $Mg^{\times\times}$ with $:\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}:$ and $:\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}:$

Electrovalency:

No. of $\bar{e}$'s lost or gained

→ 9+ Always taken +ve

G-I Li, Na, K → 1 E.V

G-II Be, Mg, Ca → 2 E.V

G-III Al, Ga → 3 E.V

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G-15 : N, P, As → 3

G-16 : O, S, Se → 2

G-17 : F, Cl, Br → 1

{ G-II ——— G-12

d block elements → variable valency

e.g Fe → +2, +3 }

~~Ener~~

: **Favourable conditions for ionic bond:**

① Metal ② Non metal ③ M + non-metal

① $M \longrightarrow \bar{e} + M^{\oplus}$ Energy absorbed → ionization energy

② Non metal + $\bar{e} \longrightarrow X^{\ominus}$ energy Released → electron Affinity

③ M + N.M

$M^{+}_{(g)} + \bar{X}_{(g)} \longrightarrow MX_{(s)}$ → stable → so energy Released called Lattice energy.

∴ when Gaseous cations React with gaseous Anions then Energy Released called Lattice energy*

OR Energy Releases

∴ When one mole ionic compound formed by cation & Anion called Lattice energy.

NOTE → more Lattice energy Released more will be favourable / stable compound.

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conditions

- Metal → ionization energy should be less
- Non-Metal → E. Affinity should be more
- Compound → Lattice energy should be more

which is more ionic ?

Metal + non metal

M.C ↑ N.M.C ↑

Q= NaF (strong Bond, more ionic), NaCl, NaBr, NaI → more covalent.

more N.M.C ← F, Cl, Br, I → N.M.C ↓

Q= LiCl, NaCl, KCl, RbCl

LiCl: more covalent

RbCl: more ionic

Li, Na, K, Rb → M.C ↑

Properties of ionic compounds:

① physical state : → solid

Lattice compounds in 3D state.

② M.P & B.P :- v. high

③ Conductivity → Bad conductor in solid state bic ions are not free but in molten state | aquous state → become good conductor.

④ Isomerism :- → mostly in covalent compounds.

molecular formula same

Different structures

→ single NaCl → has no shape but lattice has a shape.

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There is no isomerism in ionic compounds.

but Isomorphism occur in ionic compounds.

3D same ← { similar formula
size of cation & anion nearly same

e.g NaCl MgCl

3-D structure of MgCl is same like NaCl

e.g NaF MgO

e.g NaCl KCl ✗ size ~~same~~

large difference in

⑤ TYPE OF Reaction → ionic Reactions are very fast (~~10⁻⁶~~ s)

⑥ Solubility → Hydration / solvation energy

∴ If E.N diff 1.7 or >1.7
⇓ Then ionic Bond

∴ If E.N diff < 1.7
↓ covalent

Lattice energy

★ → NaCl → 72% ionic character
★ → CsF → 92% ionic character

$$Na^+_{(g)} + Cl^-_{(g)} \longrightarrow NaCl_{(s)}$$

stable

The energy released when one mole of ionic compound is formed from gaseous ions.

OR

The Amount of energy required to

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Fajan's Rule

ionic compounds has some covalent character.

★ covalent character in ionic bond is described by Fajan's Rule

→ ionic character more B.P more.

→ ionic character more solubility more

Limitation:

★ It is Qualitative law. we can not told the % age of character ionic compound

As Attraction occur electronic cloud of anion deformed due to cation called polarization of anion. sharing of electron Start → covalent character start so we can say that Any ionic compound has some covalent character

we Felt that anion is sharing the electron so covalent character is present.

covalent character depends on:

i) polarization of Anion ↑ C.C ↑

ii) polarizing power ↑ C.C ↑ of cation

↓

These two Factors described by Fajans Rule.

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Cation : polarizing power

① size of cation

polarizing power ∝ 1/size of cation

here charges are dispersed → polarizing power is less.

here charge density has increased so its polarizing power is more.

∴ size of cation ↓ p. power ↑

② charge of cation: ↑ p. power ↑

e.g $Li^+ > Na^+ > K^+ > Pb^+$

more polarizing power bic size is less

$Be^{2+} > Mg^{2+} > Ca^{2+} > Sr^{2+}$

polarizing power ∝ charge on cation

e.g $Na^+ < Mg^{2+} < Al^{3+}$

size Factor not more affect so charge Factor will affect

③ Pseudo Noble gas configuration (→ like Noble gas)

ns^2, np^6 → noble gas → 8 $\bar{e}$ in Last Shall

Ne	Ar	Kr
$2s^2, 2p^6$	$3s^2, 3p^6$	$4s^2, 4p^6$

→ ns^2, np^6, nd^{10} → pseudo noble gas configuration

↓ This configuration is Just like Noble gas ($18\bar{e}$ valence shall)

NOTE The cations which have pseudo noble gas configuration ⇒ ~~polarisation~~ polarizing power ↑ Covalent C. ↑

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Example

$_{29}Cu \longrightarrow [Ar]\ 3d^{10}, 4s^1$

$_{29}Cu = 1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^1$

$Cu^{+} = 1s^2, 2s^2, 2p^6, \boxed{3s^2, 3p^6, 3d^{10}}$

so cuper cation has more polarizing power and more covalent character.

- ✓ $Cu^{+} \rightarrow 3s^2, 3p^6, 3d^{10}$
- ✓ $Ag^{+} \rightarrow 4s^2, 4p^6, 4d^{10}$
- ✓ $Au^{+} \rightarrow 5s^2, 5p^6, 5d^{10}$

→ has more covalent character

$_{30}Zn = 1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^2$

$Zn^{2+} = 1s^2, 2s^2, 2p^6, \boxed{3s^2, 3p^6, 3d^{10}}$

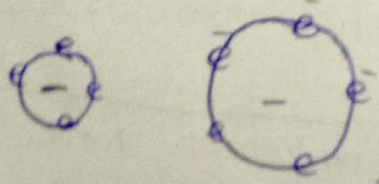
- ✓ $Zn^{2+} \Rightarrow 3s^2, 3p^6, 3d^{10}$
- ✓ $Cd^{2+} \rightarrow 4s^2, 4p^6, 4d^{10}$
- ✓ $Hg^{2+} \rightarrow 5s^2, 5p^6, 5d^{10}$

→ more covalent character

Anion: → polarization

① size of Anion:

size of anion ∝ polarization



size ↑ C.C ↑

bic in large size electrons are dispersed and easily attracted by cation

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② Charge of Anion:

charge on anion ∝ polarisation

charge ↑ C. character ↑

Q.1 : Which one has more covalent character in ionic compound: ?

NaCl > KCl > RbCl

NaCl: cation size is less → so more polarizing power → so more covalent character.

RbCl: cation size is more

Q.2 NaCl < NaBr < NaI

NaCl: less Anionic size so less covalent character

NaI: Anion size is more so more covalent character

Applications:

★ Solubility:

* covalent chacter ↑ solubility ↓

→ covalent bond is ~~strong~~ weak than ionic.

∴

M.P & B.P ↓

∴ so,

* covalent character ↑ M.P & B.P ↓

★ colour imparting nature:

* covalent chacter ↑ colour imparting nature ↑

Q.1: Which will have higher melting point?

$BeF_2 < MgF_2$

BeF_2: size less, more covalent character, so ~~higher~~ lower M.P

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Q.2: which one has more M.P?

$NaCl > CuCl$

Follow pseudo configuration so more c.c so less M.P

Q.3: Which is more soluble?

$Fe(OH)_3 < Fe(OH)_2$

Fe^{3+} ↓ charge more

c.c ↑ → solubility less

Fe^{2+}

Q.4: which is more soluble?

$Ag_2O > Ag_2S$

↓ size more → more covalent character so less solubi

Q.5: Which one has darkest colour?

$AgF < AgCl < AgBr < AgI$

↓ size more more c.c ↑ so colour impa ting more so darkest.

Q.6 which one has yellow and white colour

$PbCl_2$ ↓ white

PbI_2 ↓ more size more c.c more imparting colour so this will be yellow

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2) VBT

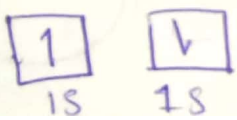
Lewis theory fails to tell about the shape and Geometry. so need of VBT occur. This gave the concept of σ & π bond.

- Actually how bond is formed told by VBT.
- It Also tells about the overlapping of Atomic orbitals and covalent bond is formed.
- This theory was introduced by (pauling & slater) in 1916.

postulates: (conditions of formation of covalent bond:)

(i) Covalent Bond is formed by overlapping of Atomic orbitals.

(ii) Only half filled orbitals with $\bar{e}$ of opposite spin, should overlap



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(iii) overlapping must be less than 50% bic of overlapping greater Nucli will come so much closed that Repulsion will occur.

(iv) Extent of overlapping decides by stiength of bond.

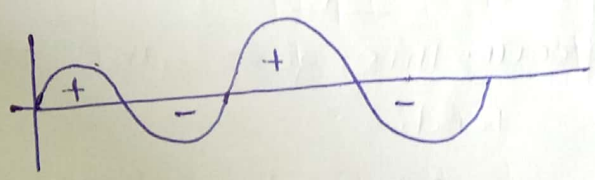
(v) Two types of overlapping are possible

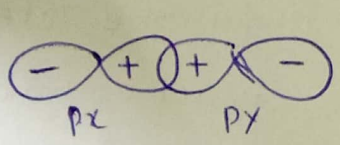
a) Axial overlapping / Head-on overlapping
↓
σ-bond formed

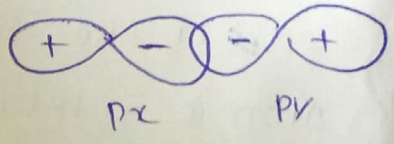
b) parallel overlapping / sidewise overlapping
↓
π-bond formed

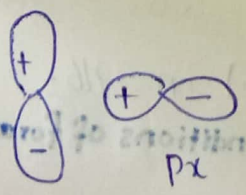
(vi) The overlapping orbitals must have same sign.

→ orbital is wave



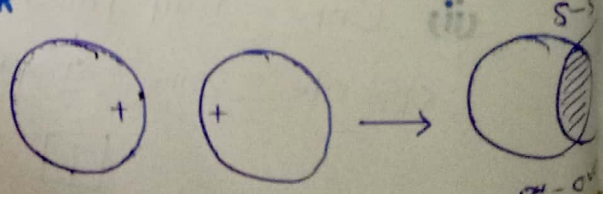






Px → here bond formation is not possible bic both's orientation is different

1. ★ Axial overlapping: ★



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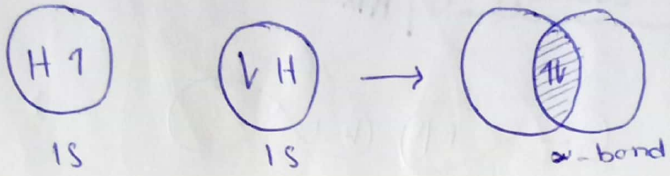
S-S overlapping: is always axial bic S orbital is spherical symmetric (non directional)

→ S orbital can never form π-bond.

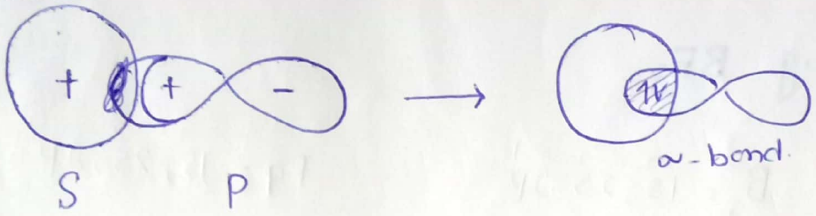
e.g H_2

H
$1s^1$
[1]

H
$1s^1$
[1]
$\longrightarrow H_2$



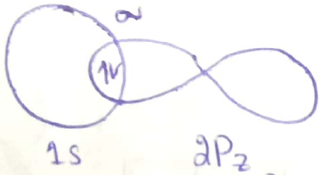
S-P orbital



e.g H-F

H
$1s^1$
[1]
1s

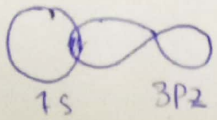
F
$1s^2, 2s^2, 2p^5$
[1↓] [1↓] [1↓ | 1↓ | 1]
$1s^2$ $2s^2$ 2p



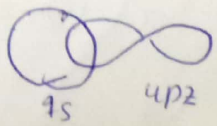
→ may be 2py, 2px

There is no condition for 2pz, 2py, 2px but generally people use $2p_z$ of one orbital has to be Reactt of 2p.

H-Cl



, **H-Br**



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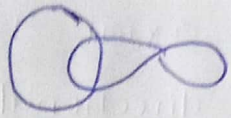
H-I



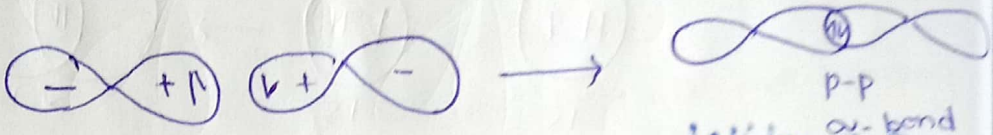
1s Sp2

Q: which bond has more B.E ?

more the shall close to the nucleous bond is strong and ~~less~~ more will be B.E

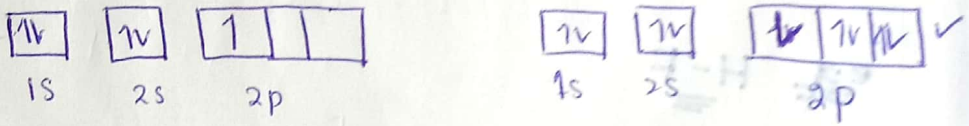
1s-2p > 1s-3p > 1s-4p > 1s-5p

P-P overlapping | Axial

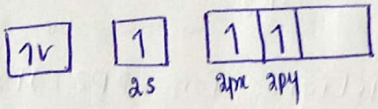


e.g BF_3

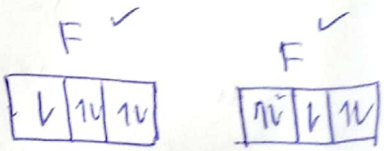
$B_5 = 1s^2, 2s^2, 2p^1$ $Fq = 1s^2, 2s^2, 2p^5$



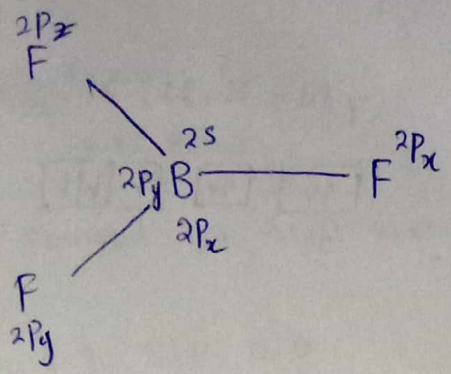
There are 3 Fluorine Atoms. Boron has only one unpaired electron that can React to only one Fluorine Atom. So For this in Boron excitation of electron occur As;

excited 

Now Boron can React with All three Fluorine Atoms.



→ s orbital will overlap to 2Pz and others $P_x - P_x$ and $P_y - P_y$ overlap.



NOTE:
1st bond b/w two atoms Always will be σ-bond.

H_2O

This is not the example of p-p overlapping

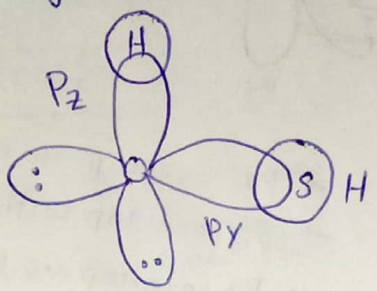
$_8O = 1s^2, 2s^2, 2p^4$

↑↓	↑↓	↑↓	↑	↑

H H

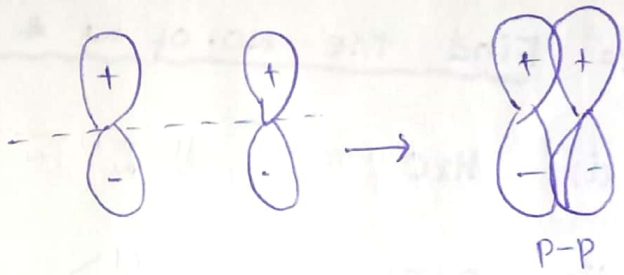
$1s^1$ $1s^1$

↑	↑



2. Parallel Overlapping

P-P overlapping



e.g O_2

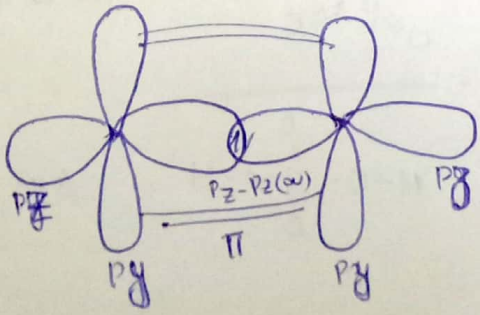
$(O=O)$

$_8O = 1s^2, 2s^2, 2p^4$

		x	y	z
↑↓	↑↓	↑↓	↑	↑

$_8O = 1s^2, 2s^2, 2p^4$

		x	y	z
↑↓	↑↓	↑↓	↑	↑



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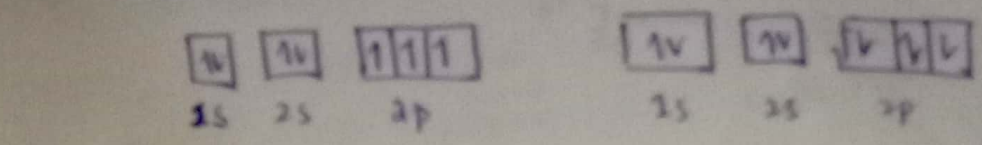
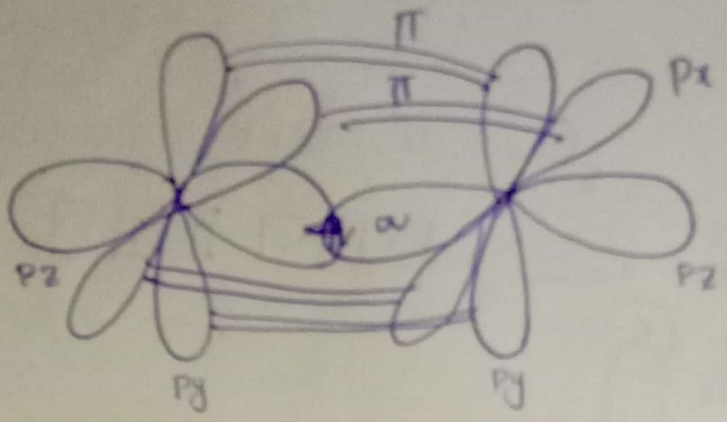
N_2

$N \equiv N$

$_7N = 1s^2, 2s^2, 2p^3$ $\quad$ $_7N = 1s^2, 2s^2, 2p^3$





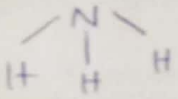
→ Px overlap with Px
→ Py overlap with Py
→ Pz overlap with Pz

NOTE

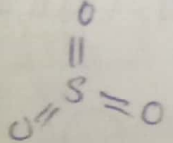
σ-bond shows more overlapping than π-bond

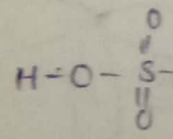
Q: Find the no. of σ & π bonds:

(i) H_2O $\quad$ $H-\underset{\sigma}{O}-\underset{\sigma}{H}$ $\quad$ 2σ

(ii) NH_3 $\quad$  $\quad$ 3σ

(iii) C_2H_2 $\quad$ $H-C\equiv C-H$ $\quad$ 3σ & 2π

(iv) SO_3 $\quad$  $\quad$ $3\sigma + 3\pi$

(v) H_2SO_4 $\quad$  $\quad$ $6\sigma + 2p$

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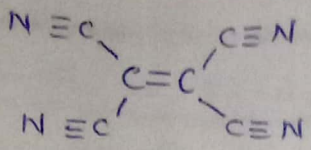
(vi) $C_2(CN)_4$



9 σ & 9 π

Difference

σ - Bond	π - bond
(i) Formed by Axial overlapping	(i) Formed by parallel overlapping
(ii) S-S, S-P, P-P	(ii) P-P, P-d, d-d
(iii) extent of overlapping is more so stronger bond, B.E ↑ B.length ↓, more stable Bond	(iii) vise versa
B.E > 80 Kcal/mol	B.E ≈ 65 Kcal/mol
(iv) Only one sigma bond can be formed b/w two atoms.	(iv) 1 or 2 π bonds can be formed.
) σ bond can be formed alone.	(vi) π- is formed with σ-bond
) in σ bond → Rotation is possible.	(vi) In π-bond Restricted Rotation is present mean Rotation is not possible

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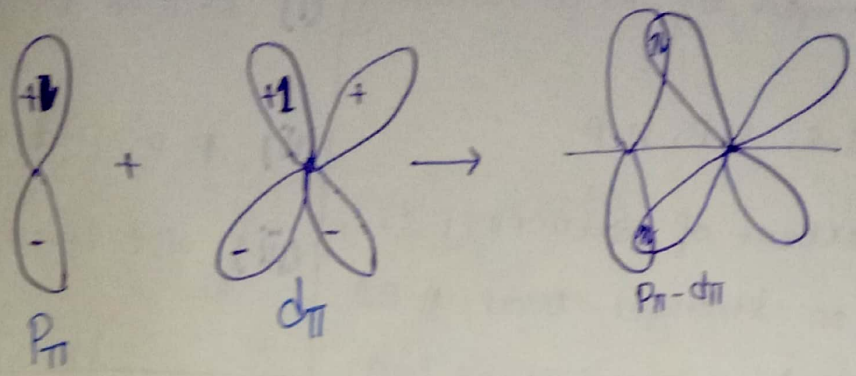
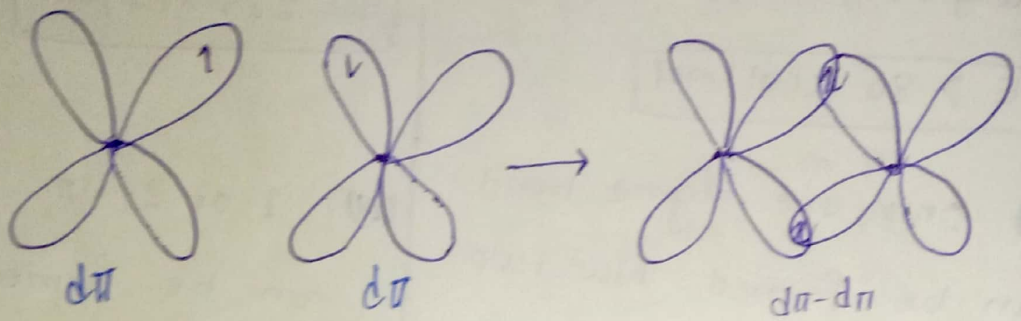
π Bond:

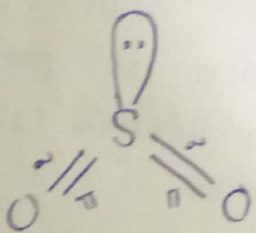
: $P_\pi - d_\pi$ overlapping: & $d_\pi - d_\pi$ overlapping



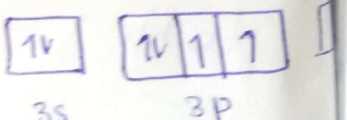


Strong overlapping in $P_\pi - P_\pi$ than $P_\pi - d_\pi$ & $d_\pi - d_\pi$

Q.1: How many $P_\pi - P_\pi$ & $P_\pi - d_\pi$ bond are in SO_2 ?

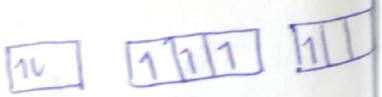


$_{16}S = 1s^2, 2s^2, 2p^6, 3s^2, 3p^4, 3d^0$

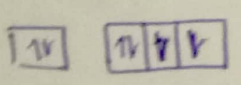


excited state

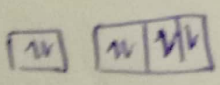
$_{16}S =$



$_8O = 1s^2, 2s^2, 2p^4$



$_8O = 1s^2, 2s^2, 2p^4$



Ans $2p_\pi - 3p_\pi$, $2p_\pi - 3d_\pi$

↓ 1-bond ↓ 1-bond

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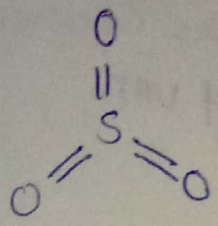
Q.2 How many $P_\pi - P_\pi$ & $P_\pi - d_\pi$ bonds are in SO_3?

Ans:



one $2P_\pi - 3P_\pi$

two $3d_\pi - 2P_\pi$

$_{16}S = 1s^2, 2s^2, 2p^6, 3s^2, 3p^4, 3d^0$

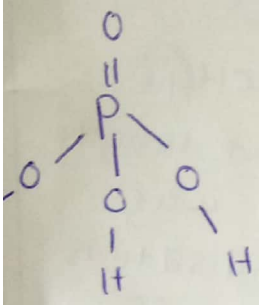
S = [1] [1 1 1] [1 1 | | |]
3s 3p 3d

$_8O$ = [1↑↓ 1 1]
2p

$_8O$ = [1↑↓ 1 1]
2p

$_8O$ = [1↑↓ 1 1]
2p

Q.3: Find no. of $P_\pi - P_\pi$ & $P_\pi - d_\pi$ in H_3PO_4?



$_{15}P = 1s^2, 2s^2, 2p^6, 3s^2, 3p^3, 3d^0$

[1] [1 1 1] [1 | | | |]
3s 3p 3d

$_8O$ = [1↑↓ 1 1]

$_8O$ = [1↑↓ 1 1]

$_8O$ = [1↑↓ 1 1]

$_8O$ = [1↑↓ 1 1]

$_8O$ = [1↑↓ 1 1]

H = [ ]

Ans ≡

$2P_\pi - d_\pi$ ↓ ① , $P_\pi - P_\pi$ ↓ 0 ≡

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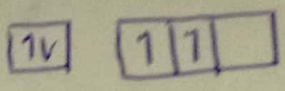
3): HYBRIDISATION :→ gives Geometry

↳ expansion of VBT

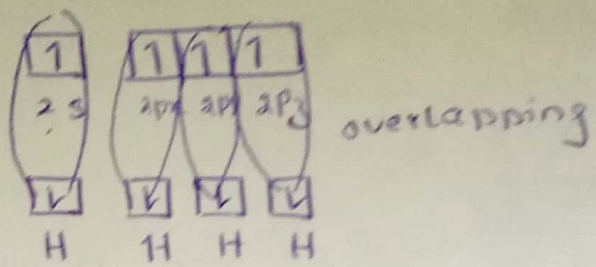
Methane CH_4 VBT

$C_6 = 1s^2, 2s^2, 2p^2$



excited state

$C_6 =$



These four ~~bonds~~ orbitals of CH_4 are different

Why we need Hybridisation?

Reason is that All 4 bonds of CH_4 are equalent in All respects Bond length same, Bond Energy same this was not told by VBT so Hybridisation was necessary

Atomic orbitals of same or nearly same energy intermix to give new orbitals of exactly same energy called Hybridisation

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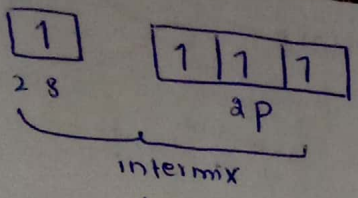
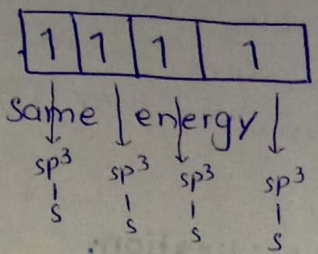
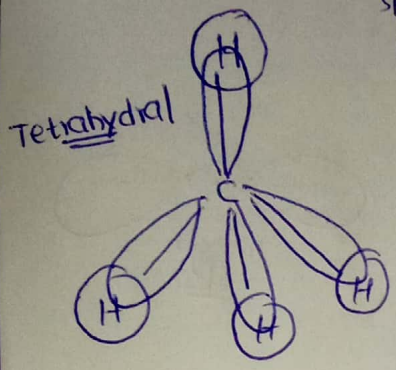
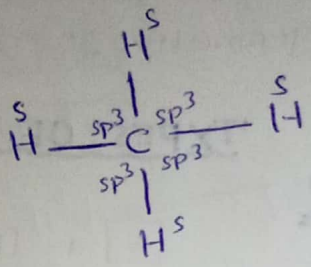


→ All four have different energy according to VBT



→ Hybridisation





NOTE
Hybridization gives the Geometry -

Main points

1) Intermixing of Atomic orbitals of same or nearly same energy (2s & 2p) to give new orbitals of exactly same energy

2)
- *Half filled orbitals
- * Empty Orbitals
- * Fullfilled orbits

→ All show Hybridisation

↓ when lone pair are present.

3) The no. of Hybrid orbitals = no. of intermixing orbitals

4) Concept of Hybridisation is only for σ bond and lone pair.

NOTE : It's no Relation with π-bond.*

5) Hybrid orbitals are named after parent orbitals

1s □ + 1p □ = □ □ (sp sp)

1s □ + 3p □□ = sp3 sp3 sp3 sp3

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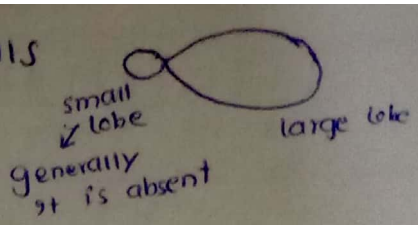
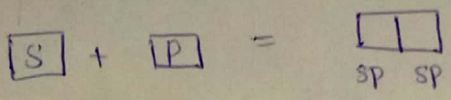
6) Shape of hybrid orbitals

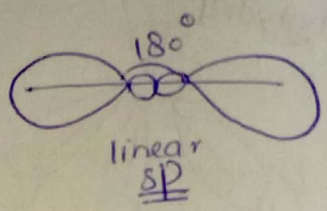


7) The Hybrid orbitals orientate that repulsion btw them is mimum so that stabity more due to this repulsion they generate a geometry.

TYPES OF HYBRIDISATION:

SP



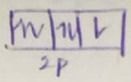


e.g BeF_2 F – Be – F

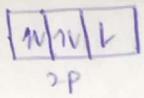
$_4Be = 1s^2, 2s^2, 2p^0$

This can React with the Fillorine so excitation will occur

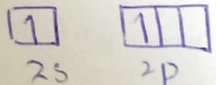
$_9F = 1s^2, 2s^2, 2p^5$



$_9F = 1s^2, 2s^2, 2p^5$

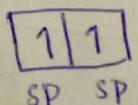


$Be = 1s^2, 2s^2, 2p^0$

$=$  → intermix

There is still problem s-orbital can not overlap with p-orbital so intermixing is important.

*



intermixed

Now they can React

so Geometry will be sp → linear

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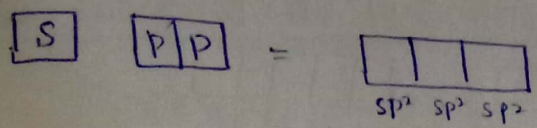
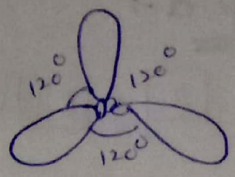
sp^2

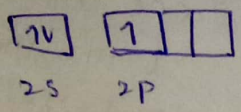


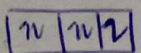


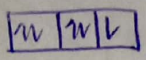
triangular planer

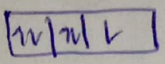
Example BF_3

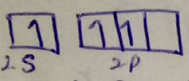
$B = 1s^2, 2s^2, 2p^1$



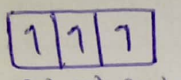
$_9F =$ 

$F =$ 

$F =$ 

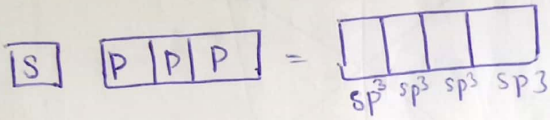
Excited state = 

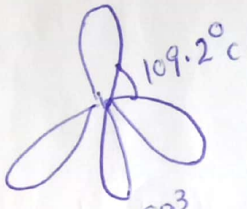
Not React S with P so intermixing



Now can overlap so we called sp^2 Geometry called triangular planner.

sp^3





sp^3 (Tetrahydral)

Example

CH_4

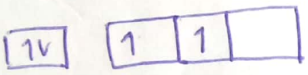
$_6C = 1s^2, 2s^2, 2p^2$

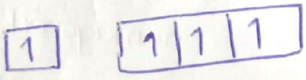
$H =$

$H =$

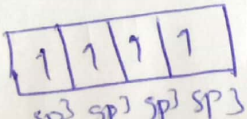
$H =$

$H =$

$=$ 

$=$ 

intermix

$=$ 

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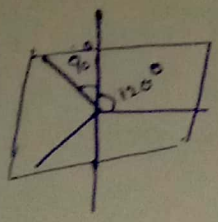
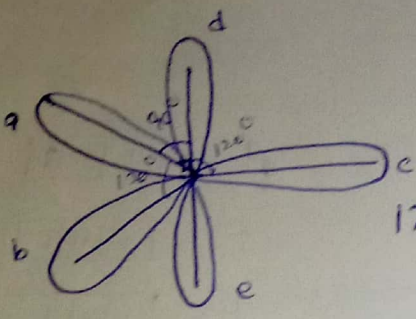
sp^3d →

[S] + [P|P|P] + [d] = [| | | |]

sp^3d sp^3d sp^3d sp^3d sp^3d





Trigonal Bipyramidal

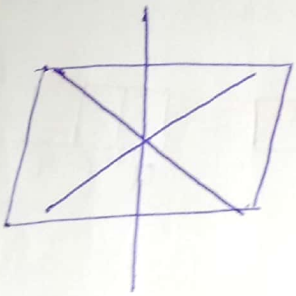
120° ← ★ a, b, c → orbitals are in the same plane

90° ← ★ d → is above the plane
★ e → below the plane.

Example = PCl_5

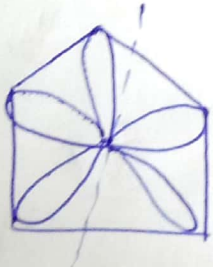
sp^3d^2 → octahydral

[S] [P P P] [d d]



Example = SF_6

sp^3d^3



pentagonal Bipyramidal

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✓ : How to Find out Hybridisation:

Two ways

By Structure (single bond + lone pair)

By Formula

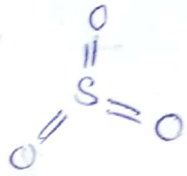
(I) : By Structure:

Z = no. of σ bonds + l.p of central Atom

Z =	Hybridization
2	sp → linear
3	sp^2 → triangular planar
4	sp^3 → tetrahydral
5	sp^3d → trigonal Bipyramidal
6	sp^3d^2 → octahydral
7	sp^3d^3 → pentagonal Bipyramidal

NOTE: ... central Atom ... Hybridization

→ SO_3:



Z = 3 + 0

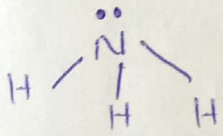
Z = 3 ⇒ sp^2

→ H_2O:

Z = 2 + 2 = 4 (sp^3)

★ tetrahydral

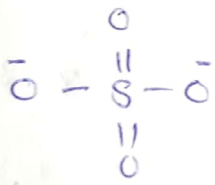
→ NH_3



Z = 3 + 1 = 4 (sp^3)

tetrahydral

→ S in SO_4^{2-}



Z = 4 + 0 = 4 (sp^3)

(tetrahydral)

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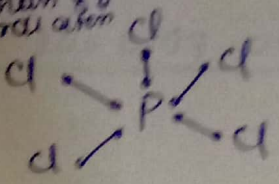
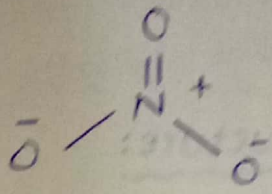
→ P in PCl_5 → superscript means bic more than 8 of central atom



$Z = 5 + 0 = 5\ (sp^3d)$

Trigonal Bipyramidal

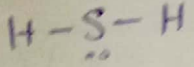
→ N in NO_3^{1-}



$Z = 3 + 0 = 3\ (sp^2)$

(triangular planner)

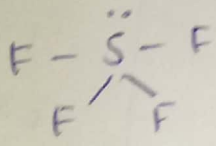
→ H_2S



$Z = 2 + 2 = 4$

tetrahydral

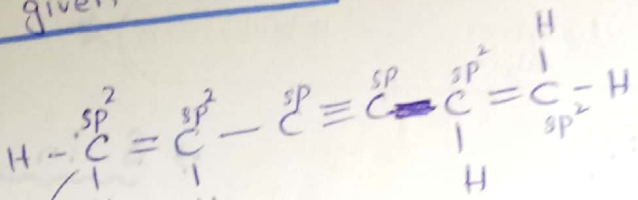
→ SF_4



$Z = 4 + 1 = 5$

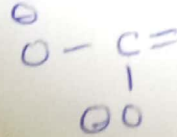
trigonal Bipyramidal

Q: Find Hybridization of All C atoms in the given molecule ?



$Z = 3 + 0 = 3 \rightarrow sp^2$

→ C in CO_3^{2-}



$Z = 3 + 0 = 3$

trigonal planner

Sometimes we donot know the structure OF the compounds so we use easy & another method

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(II) Super trick Method (By Formula)

$$Z = \frac{1}{2}\left(\text{no. of v. electron on central Atom} + (\text{-ve charg}) - (\text{+ve charge}) + \text{no. of monovalent Atoms} \right)$$

H, F, Cl, Br

Examples

N in NH_3

$Z = \frac{1}{2}(5+3) = \frac{1}{2}\times 8 = 4 \rightarrow sp^3 \rightarrow$ tetrahydral

H_2O

$Z = \frac{1}{2}(6+2) = 4 \rightarrow sp^3 \rightarrow$ tetrahydral

CO_3^{2-}

$Z = \frac{1}{2}(4+2) = 3 \rightarrow sp^2 \rightarrow$ triangular planer

NO_3^{-1}

$Z = \frac{1}{2}(5+1) = 3 \rightarrow sp^2 \rightarrow$ triangular planner

SiF_4:

$Z = \frac{1}{2}(4+4) = 4 \rightarrow sp^3 \rightarrow$ tetrahydral

SF_4:

$Z = \frac{1}{2}(6+4) = 5 \rightarrow sp^3d \rightarrow$ ~~triangular planner~~ trigonal Bipyramidal

XeO_2F_2

$Z = \frac{1}{2}(8+2) = 5 \rightarrow sp^3d \rightarrow$ trigonal Bipyra-middle

XeF_4 $Z = \frac{1}{2}(8+4) = 6 \rightarrow sp^3d^2 \rightarrow$ octahydral

* ——— *

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4) VSEPR Theory: → presented By Nyholm & Gillespie

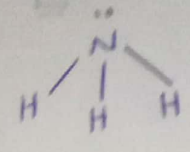
This tells us about the exact shape of molecule which is not told by the hybridization (told the geometry of molecule)

∴ NOTE: Geometry and shapes are not same

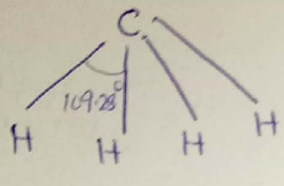
We can find out the bond pairs and lone pairs by Z value.

Example

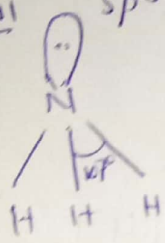
NH_3 = $Z = \frac{1}{2}(5+3) = 4$ ↓ Surrounding Atoms are 3 → so bond pairs are three and one will be lone pair.



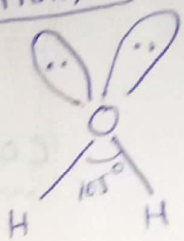
tetrahydral sp^3



tetrahydral sp^3



tetrahydral sp^3



★ Hybridization and VBT says that bond angle blw Atoms of All three compounds CH_4, NH_3, H_2O should be same 109.28° due to same bonds. But VSEPR says that due to lone pairs then Hybridisation Fails and Angles changed so in NH_3 angle is 107° and in H_2O angle is 105°. So This VSEPR theory was needed.

Diff.

★ Geometry: Arrange of b·pairs and lone pairs

In this we see both things

★ Shape: (B·P) Arrangement of Atoms around central Atom.

in shape no Relation with lone pairs if we neglect the lone pair then see

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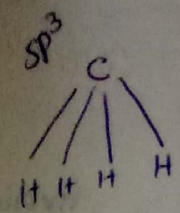
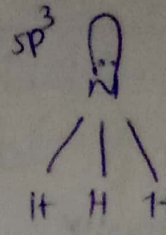
the structure. then we can determine the shape



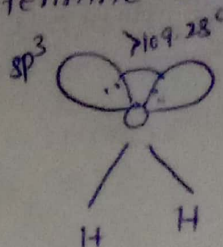
Shape ⇒ tetrahydral

Geometry ⇒ tetrahydral



Shape = pyramid

Geometry = tetrahydral



Shape = angular/ bent / V-shaped

Geometry = tetrahydral

Why angle changed this is explained by VSEPR.

Electron pair = lone pair + bond pair

NOTE: in different electron pairs Bond angle different due to Repulsion OF lone pairs.

∴ in NH_3 → lone pair repels the ~~more~~ Hydrogen more and push the Hydrogen below. and bond angle decrease upto 107°.

∴ In H_2O → Repultion blw two lone pairs is more due to this angle increases and blw Hydrogen Angle more decreases that is 105°

Main points

① Electron pairs are always Repelling eah other & trying to remain apart.

② Diff. ē pairs have different order OF repulsion. Repulsion ~~is~~ order

$$L.P - L.P > l.P - b.P > b.P - b.P$$

③ When lope pair is zero then Geometry is shape

Else geometry ≠ shape ~~Shape~~

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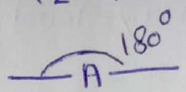
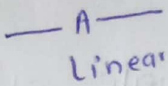
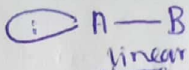
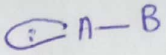
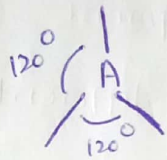
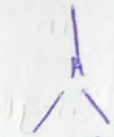
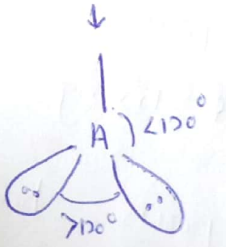
④ Geometry depends upon (B.P & L.P) Z value.

⑤ Shape depends upon surrounding Atoms (B.P)

Z	B.P	L.P	Geometry (Z = L.P + B.P)	Shape (B.P)	Hybridization
2	2	0	 Linear	 Linear	SP
2	1	1	 linear ~~no shape~~ Geometry	 no shape	SP
3	3	0	 trigonal planer	 trigonal planer	sp^2
3	2	1	trigonal planer	Bent angular	sp^2
3	1	2	~~no shape~~ trigonal planer 	no regular shape	sp^2

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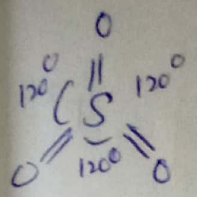
Q: Find no. of l.p, hybridization, geometry, shape

SO_3

$Z = \frac{1}{2}(6) = 3$ (l.p + B.P)



∴ lone pair = 0

Hybridization = sp^2

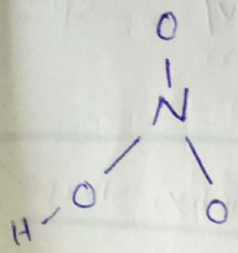
Geometry = trigonal planer

Shape = trigonal planer

HNO_3

$Z = \frac{1}{2}(5 + 1) = 3$ (lone pair + Bond pair)

(1 ← mono-valent)



lone pair = 0

Geometry = trigonal planer

Shape = trigonal planer

Hybridization = sp^2

NO_3^{1-}

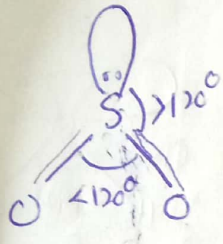
$Z = \frac{1}{2}(5 + 1) = 3 \rightarrow sp^2$

l.p = 0

Shape & Geometry = trigonal planer

SO_2

$Z = \frac{1}{2}(6) = 3$ sp^2



lone pair = 1

Geometry = trigonal planer

Shape = Bent/angular/V-shaped

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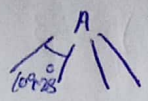
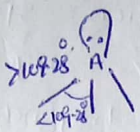
Z	B.P	L.P	Geometry	Shape	Hybridization
4	4	0	tetrahydral 	tetrahydral	sp^3
4	3	1	 tetrahyral	pyramidal	sp^3
4	2	2	tetrahydral	Bent/V/ angular	sp^3

Q: Find No. of L.P, Hybridisation, Geometry, shape ?

NH_3

$Z = \frac{1}{2}(5+3) = 4 \rightarrow sp^3$

Geometry = tetrahydral

lone pair = 1

shape = pyramidal

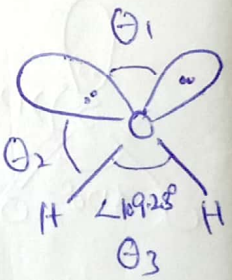
H_2O

$Z = \frac{1}{2}(6+2) = 4 \rightarrow sp^3$

Geometry = tetrahydral

lone pain = 2

shape = Bent | Angular



$\theta_1 > \theta_2 > \theta_3$

↓

Here no Regular tetrahydral angle

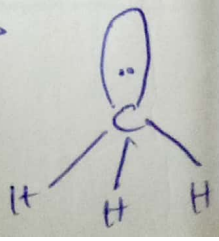
$CH_3^{\ominus}$

$Z = \frac{1}{2}(4+3+1) = 4 \rightarrow sp^3$

Geometry = tetrahydral

lone pair = 1 lone pair

Shape = pyramidal



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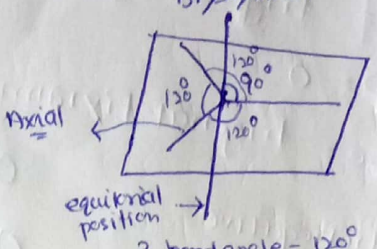
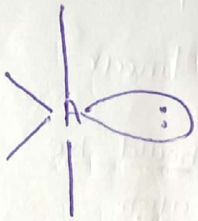
Z	B.P	L.P	Geometry	shape	Hybridization
5	5	0	trigonal Bipyrmidal	trigonal Bipyramidal → more electronegative Atom occupy equitorial position	sp^3d



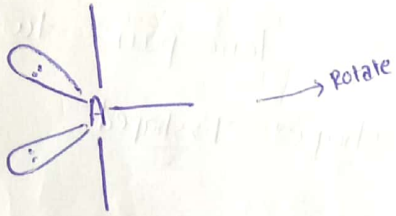
3 bond angle = 120°

6 bond angle = 90°

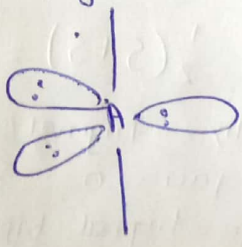
5	4	1	Tigonal Bipyramidal → L.p one placed at axial position bc lone pair is larger	see-saw جھولا جیسا	sp^3d



5	3	2	Trigonal Biyramidal	T→shaped	sp^3d



5	2	3	trigonal Bipyramidal	linear shape	sp^3d



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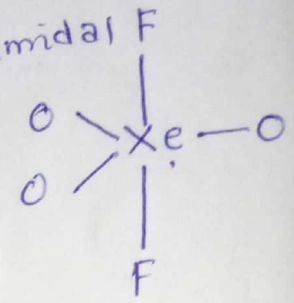
Q: Find:

XeO_3F_2 $Z = \frac{1}{2}(8+2) = 5 \rightarrow sp^3d$

Geometry = trigonal Bipyramidal

l.p = 0

shape = trigonal Bipyramidal



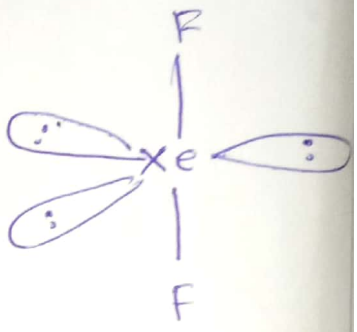
NOTE: More electronegative Atom should be on Equitorial position.

XeF_2 $Z = \frac{1}{2}(8+2) = 5 \rightarrow sp^3d$

Geometry = trigonal Bipyramidal

lone pair = 3

shape = linear



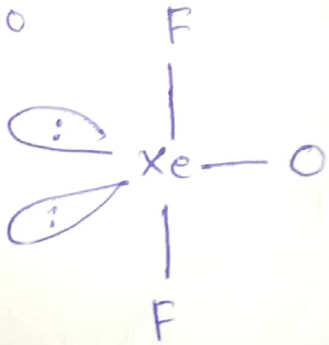
→ lone pairs should be on Axial position

$XeOF_2$: $Z = \frac{1}{2}(8+2) = 5 \rightarrow sp^3d$

Geometry = trigonal Bipyramidal

lone pair = two

shape: T-shaped



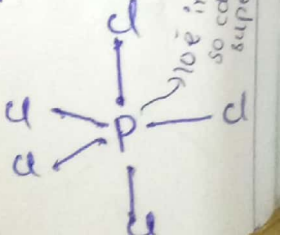
PCl_5: $Z = \frac{1}{2}(5+5) = 5 \rightarrow sp^3d$

↙ super octet molecule

Geometry = trigonal Bipyramidal

lone pair = 0

Shape = trigonal Bipyramidal


d
d
P
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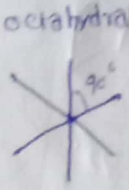
d

Z	B.P	L.P	Geometry	shape	Hybri:
6	6	0	octahydral  All angles are at 90° 6 → 90° angles	octahydral e.g SF6	sp^3d^2
6	5	1	octahydral → Rotate	square pyramidal	sp^3d^2
6	4	2	octahydral	square planer e.g XeF4	sp^3d^2

SF6

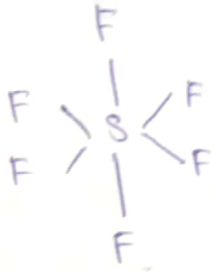
supercoctet molecule

$Z = \frac{1}{2}(6+6) = 6 \rightarrow sp^3d^2$

Geometry = octahydral

lopair = 0

Shape = octahydral



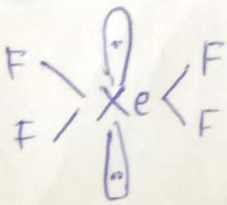
XeF4

$Z = \frac{1}{2}(8+4) = 6 \rightarrow sp^3d^2$

Geometry = octahydral

lone pair = 2

Shape = square planner



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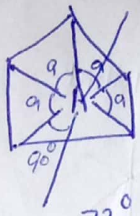
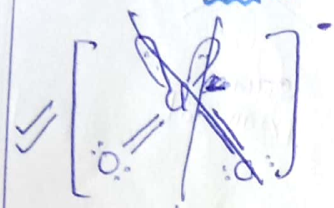
Z	B.P	L.P	Geometry	Shape	Hybridiz
7	7	0		pentagonal Bipyramidal e.g ICl_7	sp^3d^3

$5 \rightarrow a = 72^0$

Out of plane = 10 angle = 90^0

pentagoal Bipyramidal

ClO_2^-:



~~$Z = \frac{1}{2}(7+0+1) = 4 \rightarrow sp^3$~~

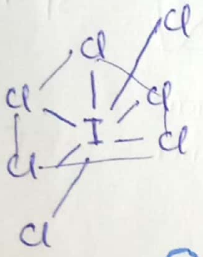
~~lone pair = 2~~

~~Geometry = pentagonal Bipyramidal~~ ~~tetrahydral~~

~~Shape = Bent~~

superoctet molecule

ICl_7:



$Z = \frac{1}{2}(7+7) = 7 \rightarrow sp^3d3$

Geometry = pentagonal Bipyramidal

lone pair = 0

Shape = pentagonal Bipyramidal

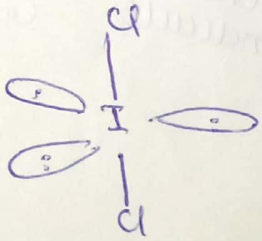
ICl_2^-

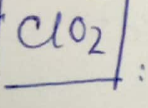
$Z = \frac{1}{2}(7+2+1) = 5 \rightarrow sp^3d$

Geometry = trigonal Bipyramidal

lone pair = 3

Shape = linear

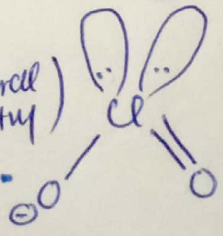


ClO_2^- 

$Z = \frac{1}{2}(7+1) = 4 \rightarrow sp^3$

Lewis structure

(tetrahydral Geometry)



$\Rightarrow$ Bent Shape

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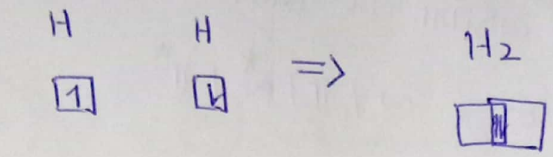
5) MOT

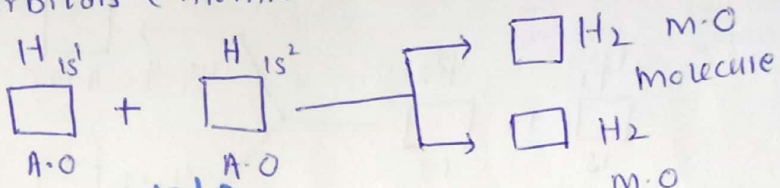
V.V. imp



This concept was given by VBT

But MOT says;

when these two ~~overlap~~ orbitals combine then form New orbitals (Atomic orbitals exist)



Why MOT was needed ?

- V.B.T does not give infamation about the orbitals OF molecules and not about magnatic nature OF molecule SO MOT was needed.
- VBT never talk about the stability OF molecules Stability Told by MOT.
- VBT does not told the correct Quantity OF bond it only told ~~or~~ Quantity OF σ & π bonds.

MOT told about Also the Bond order in Fraction

- MOT Also tells about the wave mechanics.

SO MOT was necessary

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Main points

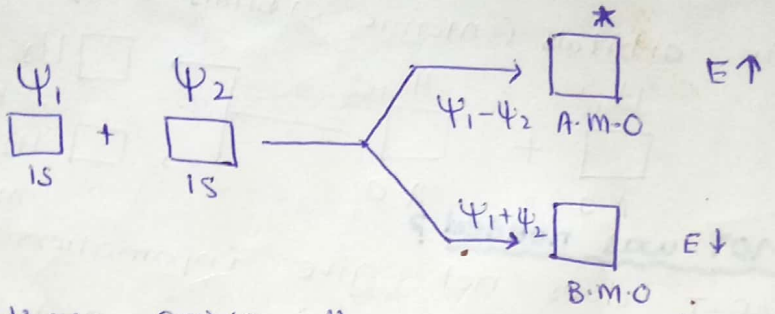
① Atomic orbital in Atoms and M.O in Molecule.

② Naming of orbital in MOT is different

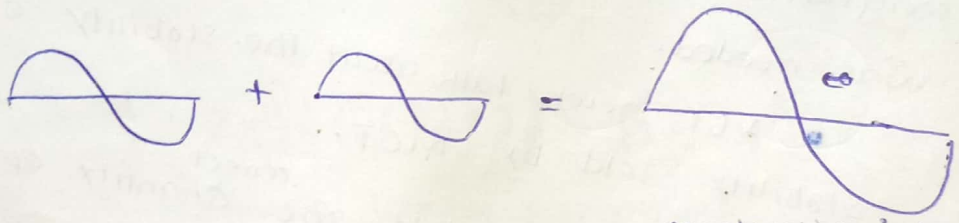
in MOT = σ / π / σ^* / π^*

③ Number of M.O formed = No. of A.O combining

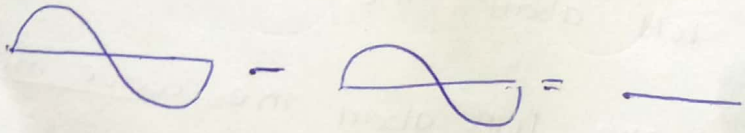
④



Schrodinger gave the name to orbital is wave Represented by ψ



constructive interferance
(Bonding M.O)
↓
Stable
↓ less E



Distructive interference
Antibonding M.O
↓
Antistable
↓
More E

⑤ Combining A.O must have nearly same energy and same shape.

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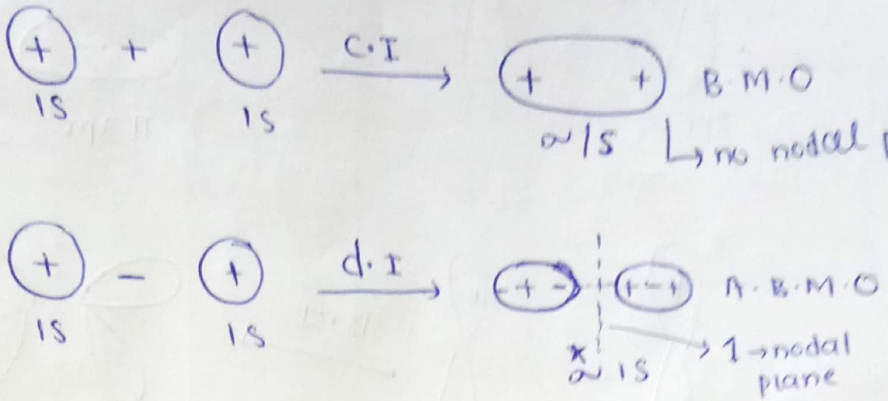
same shape = (S-S, Px-Px, Py-Py, Pz-Pz) overlapping

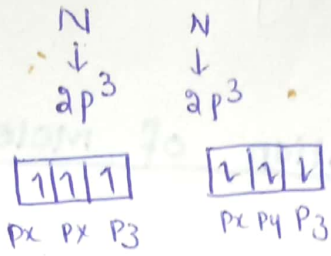
1. σ M·O: (Axial overlapping)

formed by Axial A·O interferance/overlapping

S-S



$N_2 = (N \equiv N)$



Generally we

$P_z - P_z = \sigma$

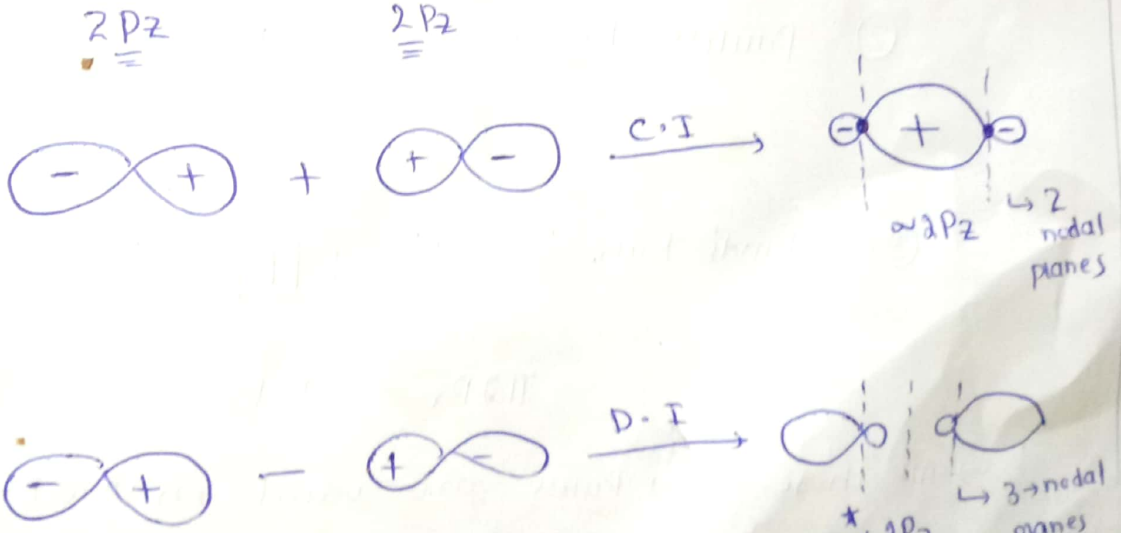
$P_x - P_x$, $P_y - P_y$ → π

NOTE

$P_x - P_y$ or $P_y - P_y$ can also form 1st σ bond

Generally say $P_z - P_z$ = σ bond

2Pz - 2Pz



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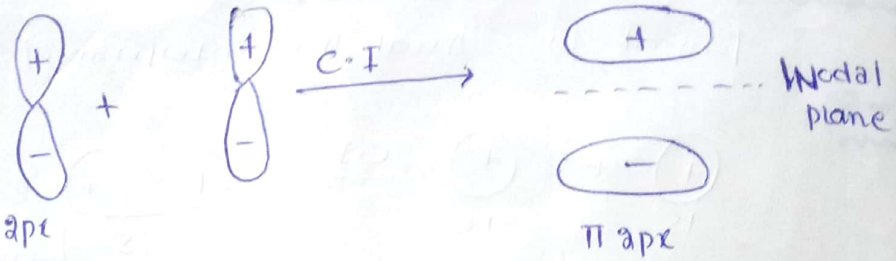
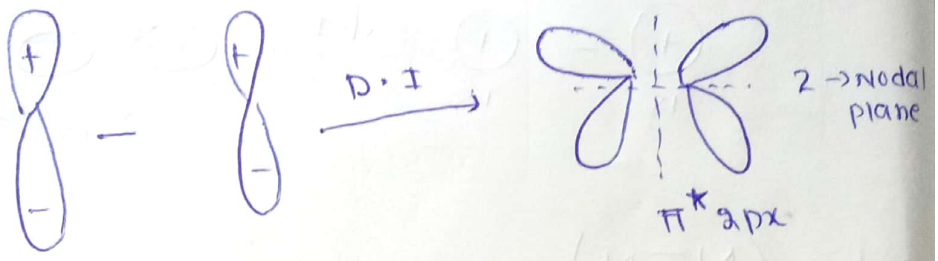
2) π. M.O (parallel overlapping)





Similarly 2py π & 2py π^* orbitals shape.

: How to do ē configuration of molecules:

: Rules:

① Aufbau Principle; → 1st ē in lower E to high

② Pauli's Principle: 1↑ M.O

③ Hund's Rule: | 1 | 1 | 1 |

$\pi 2p_x = \pi 2p_y$

→ All these 3→ Rules are valid in MOT.

④ → (N+ℓ) Rule is not valid.

⑤ → experimental order of Energies followed

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(i) Electronic configuration ≤ 14 electrons:-

: IF we have less than or equal to 14 ē:

electronic configuration

$(\sigma 1s \quad \overset{*}{\sigma} 1s), (\sigma 2s \quad \overset{*}{\sigma} 2s), (\pi 2p_x = \pi 2p_y), \sigma 2p_z$

$(\pi^* 2p_x = \pi^* 2p_y), \sigma^* 2p_z$

H_2 $(2\bar{e})$ $(H\text{-}H)$

$\sigma 1s^2$. $B.O = \frac{2-0}{2} = 1$

Bond order

$$B.O = \frac{N_b - N_a}{2}$$

He_2 $(4\bar{e})$

$\sigma 1s^2, \overset{*}{\sigma} 1s^2$

$B.O = \frac{2-2}{2} = 0 \rightarrow$ this molecule do not exists.

H_2^+ $(1\bar{e})$

$\sigma 1s^1$

$B.O = \frac{1-0}{2} = 0.5$

imp **Stability $\propto$ B.O**

Q: which one is more stable ?

H_2, He_2, H_2^+

$H_2 > H_2^+ > He_2$

B.O → ① 0.5 0

H_2^- : $\sigma 1s^2, \overset{*}{\sigma} 1s^1$

$B.O = \frac{2-1}{2} = \frac{1}{2} = 0.5$

Q= which one is more stable ?

H_2^+, H_2^-

$H_2^+ > H_2^-$

bic lesser A.B. ē

NOTE: if two molecules have same bond order then we will see the antibonding ē. Lesser will be the antibonding ē of molecule more will be stable.

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Bond length :

Bond length $\propto \frac{1}{B.O}$

Magnetic nature :

- paramagnetic → unpaired $\bar{e}$ → attract in M.F
- Diamagnetic → paired $\bar{e}$ → Repel in M.F

H_2 = Diamagnetic

H_2^- = paramagnetic

H_2^+ = paramagnetic

Li_2 : $(6\bar{e})$ → Diamagnetic

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2$

$(Li \equiv Li)$

$B.O = \frac{4-2}{2} = 1$

Li_2^+ : $(5\bar{e})$ → paramagnetic

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^1$ $\quad B.O = \frac{3-2}{2} = 0.5$

$Li_2^\ominus$ = $(7\bar{e})$ → paramagnetic

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^1$

$B.O = \frac{4-3}{2} = \frac{1}{2} = 0.5$

stability order:

$Li_2 > Li_2^+ > Li_2^\ominus$

(1) $\quad 0.5 \quad 0.5$

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Be_2 : $(8\bar{e})$ → Diamagnetic

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2$

$B.O = \frac{4-4}{2} = 0$ (do not exist)

B_2 : $(10\bar{e})$

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^1 = \pi 2p_y^1$

$B.O = \frac{6-4}{2} = 1$

Magnetic nature = unpaired → paramagnetic

C_2 : $(12\bar{e})$ $(\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^1, \sigma^* 2s^1)$ $\pi 2p_x^2 = \pi 2p_y^2$

(C=C) → ignore bic cancel to each other

$B.O = \frac{4-0}{2} = 2$

Diamagnetic

$(KK)(KK)^1$ $\pi 2p_x^2 = \pi 2p_y^2$

8 $\bar{e}$

N_2 : $(14\bar{e})$ → Diamagnetic

$N \equiv N$

$(KK)(KK^1)$ $\pi 2p_x^2 = \pi 2p_y^2$ $\sigma 2p_z^2$

$B.O = \frac{6-0}{2} = 3$

$N_2 \longrightarrow N_2^{\ominus}$

N_2 : $14\bar{e}$ → $15\bar{e}$

↓ will we Apply

Another configuration?

e^- derived ~ N_2 ~ bic ← NO ←

$N_2^{\ominus} = \sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2, \pi^* 2p_z^1 = \pi^* 2p_y$

$B.O = \frac{6-1}{2} = 2.5$

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$N_2^{\oplus}$ = 13 $\bar{e}$ →

Stability

$N_2 > N_2^{+} > N_2^{-}$

SHORT Cut

simp.

No. of $\bar{e}$	B.O
10	1
11	1.5
12	2
13	2.5
14	3

No. of $\bar{e}$	B.O
15	2.5
16	2
17	1.5
18	1

Q = Which has same B.O as N_2 ?

a) CN (b) CO c) O_2 (d) NO^+

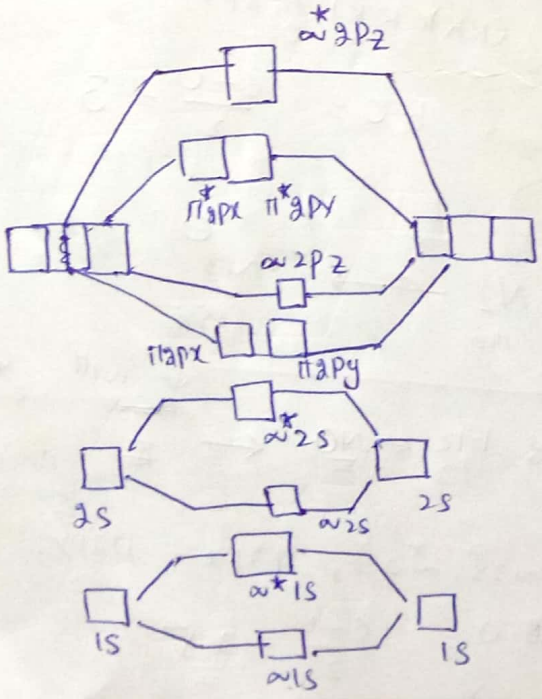
Ans CO & NO^+ bic No. of $\bar{e}$'s are 14

Energy level Diagrams:

Energy

B.M.O < A.O :نوٹ

A.B.M.O > A.O



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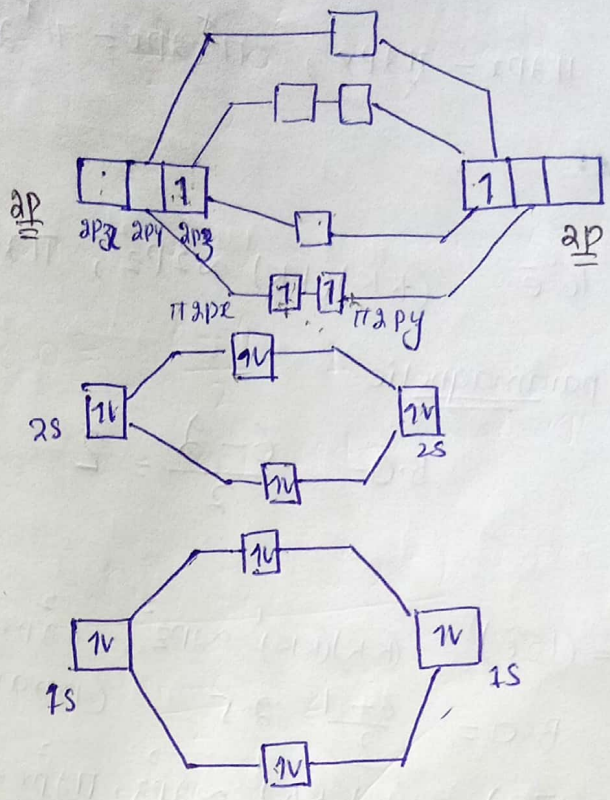
B_2 $(10\bar{e}) = \sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^1 = \pi 2p_y^1$

$_5B = 1s^2, 2s^2, \boxed{2p^1}$

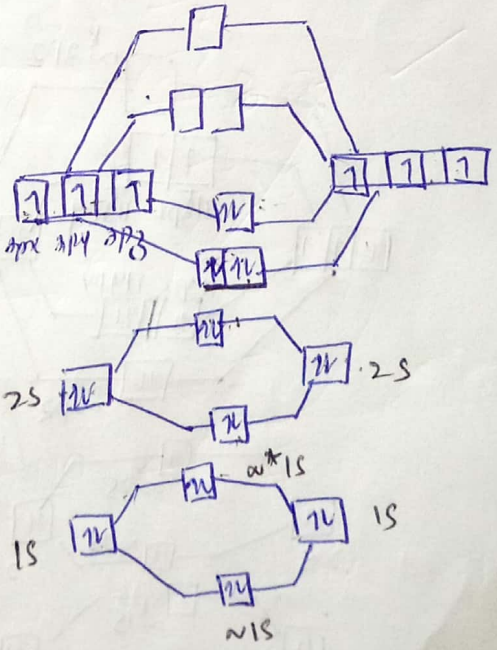


$N_2 = (14\bar{e})$: $\sigma 1s^2 < \sigma^* 1s^2 < \sigma 2s^2 < \sigma^* 2s^2 < \pi 2p_x^2 = \pi 2p_y^2 < \sigma 2p_z^2$

$_7N = 1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^1$

$_7N = 1s^2, 2s^2, 2p^3$

① E. configuration
② E-Diagram
③ Filling of $\bar{e}$
④ par/dia
⑤ B·O
⑥ E. order



$B.E = \frac{B.\bar{e} - A.B.E}{2}$

$= \frac{10-4}{2}$

$= \frac{6}{2} = 3$

$N \equiv N$

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✓ ii) : Electronic configuration: (15–20) ē

$\sigma 1s$, $\sigma^* 1s$, $\sigma 2s$, $\sigma^* 2s$, $\sigma 2pz$

$\pi 2px = \pi 2py$, $\pi^* 2px = \pi^* 2py$, $\sigma^* 2pz$

Example:

O_2: 16 ē $(KK)(KK)^1 \sigma 2pz^2$, $\pi 2px^2 = \pi 2py^2$, $\pi^* 2px^1 = \pi^* 2py^1$

(O=O) paramagnetic

$$B.O = \frac{6-2}{2} = 2$$

$O_2^+ = (15\bar{e})$ $(KK)(KK)^1 \sigma 2pz^2$, $\pi 2px^2 = \pi 2py^2$, $\pi^* 2px^1 = \pi^* 2py$

$$B.O = \frac{6-1}{2} = 2.5$$ (paramagnetic)

O_2^{+++} = (17 ē) $(KK)(KK)^1 \sigma 2pz^2$, $\pi 2px^2 = \pi 2py^2$, $\pi^* 2px^2 = \pi^* 2py^1$

$$B.O = \frac{6-3}{2} = 1.5$$ (paramagnetic)

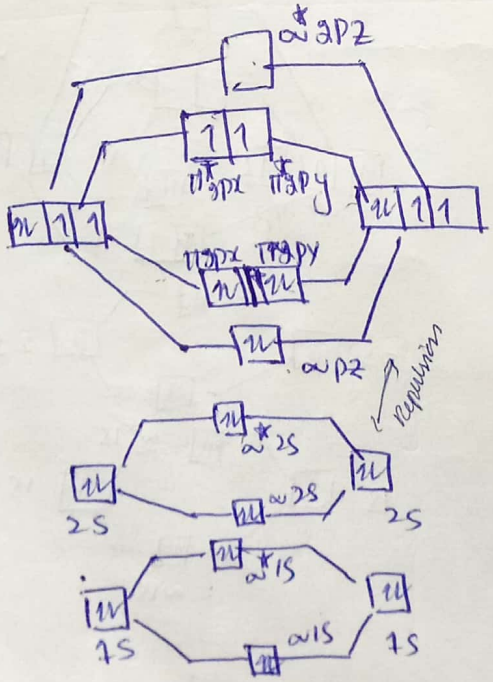
O_2^{2-}: (18 ē) $(KK)(KK)^1 \sigma 2pz^2$, $\pi 2px^2 = \pi 2py^2$, $\pi^* 2px^2 = \pi^* 2py^2$

$$B.O = \frac{6-4}{2} = 1$$ (diamagnetic)

~~General~~

O_2

$_8O = 1s^2, 2s^2, 2p^4$



paramagnetic

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Q. Compare B.O, B.L, Stability ?

a) O_2 b) O_2^- c) O_2^+ d) O_2^{2-}

Bond order

$O_2 > O_2^- > O_2^+ > O_2^{2-}$

$\downarrow \quad \downarrow \quad \downarrow \quad \downarrow$

$2 \quad 1.5 \quad 2.5 \quad 1$

Bond length

$B.L \propto \frac{1}{B.O}$

$O_2^{2-} > O_2^+ > O_2^- > O_2$

Stability

$S \propto B.O$

$O_2^{2+} > O_2^+ > O_2 > O_2^- > O_2^{2-}$

Q. Arrange in order OF B.L O—O

a) KO_2 b) Na_2O_2 c) O_2

Ans $K^+ O_2^-$ $2Na^+ O_2^{2-}$ O_2

$\downarrow \quad \downarrow \quad \downarrow$

$O_2^- \quad O_2^{2-} \quad 2$

$1.5 \quad 1$

B.O

B. Length $Na_2O_2 > KO_2 > O_2$

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V.V.V. Imp

* $N_2 = 14\bar{e}$ ≤ $14\bar{e}$ والے طریقے سے configuration کریں گے

* $N_2^- = 15\bar{e}$ $14\bar{e}$ والے طریقے سے کریں گے یا Question یہ ہے کہ اس کو configurated by ہیں۔

Ans: Yes, It is Also configurated by $14\bar{e}$ Method bic it is derived from N_2

$$N_2 + 1\bar{e} \longrightarrow N_2^{\ominus}$$

Similarly

NO: $15\bar{e}$ → This will be configurated by ~~(15-20)~~ $(15-20)\bar{e}$ → electronic configuration

NO^+: $14\bar{e}$ → This will Also be ~~configurated~~ configurated by $(15-20)\bar{e}$ Method bic ~~derived from~~ derived from NO

similarly:

$O_2 = 16\bar{e}$ → configurated by $(15-20)\bar{e}$ ~~Method~~ Method

$O_2^-(17\bar{e}),\ O_2^{2-}(18\bar{e}),\ O_2^+(15\bar{e})$,

↓ All will be configrated by ~~(15-20)~~ $(15-20)\bar{e}$ Method bic derived from O_2

{ * O_2, O_2^+, O_2^- → paramagnetic
* O_2^{2+}, O_2^{2-} → Diamagnetic }

{ N_2, N_2^{2+} → Diamagnetic
N_2^-, N_2^{2-}, N_2^+ → paramagnetic }

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